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     (FILE 'HOME' ENTERED AT 12:58:33 ON 21 OCT 2003)

     FILE 'CAPLUS' ENTERED AT 12:58:48 ON 21 OCT 2003
L1             1 S US200200159961/PN
                 SELECT L1 1 RN

     FILE 'REGISTRY' ENTERED AT 12:59:23 ON 21 OCT 2003
L2             1 S E4
L3             1 S E5
L4             1 S E6
L5             1 S E7
L6             1 S E8
L7             1 S E9
L8             1 S E10

=> save all
ENTER NAME OR (END):gellingagent/l
L# LIST L1-L8 HAS BEEN SAVED AS 'GELLINGAGENT/L'
  75% OF LIMIT FOR SAVED L# LISTS REACHED
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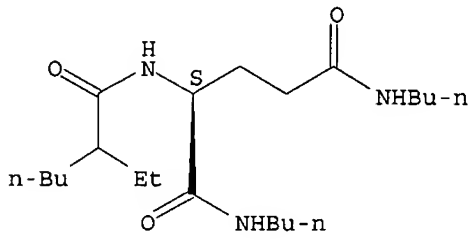
E1	1	109-73-9/BI
E2	1	111-64-8/BI
E3	1	16177-21-2/BI
E4	1	486455-65-6/BI
E5	1	486455-66-7/BI
E6	1	486455-67-8/BI
E7	1	486455-68-9/BI
E8	1	486455-69-0/BI
E9	1	486455-70-3/BI
E10	1	486455-71-4/BI
E11	1	63663-21-8/BI
E12	1	760-67-8/BI

L2 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2003 ACS on STN
RN **486455-65-6** REGISTRY
CN Pentanediamide, N,N'-dibutyl-2-[(2-ethyl-1-oxohexyl)amino]-, (2S)- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C21 H41 N3 O3
SR CA
LC STN Files: CA, CAPLUS, USPATFULL

Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

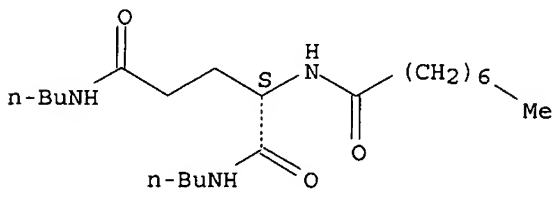
1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

=> s e5
L3 1 486455-66-7/BI

=> d

L3 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2003 ACS on STN
RN **486455-66-7** REGISTRY
CN Pentanediamide, N,N'-dibutyl-2-[(1-oxooctyl)amino]-, (2S)- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C21 H41 N3 O3
SR CA
LC STN Files: CA, CAPLUS, USPATFULL

Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

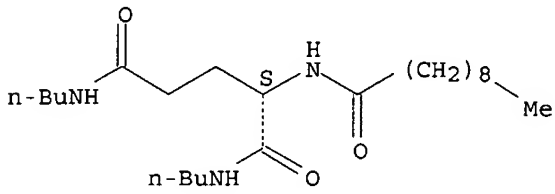
1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

=> s e6
L4 1 486455-67-8/BI

=>
=> d

L4 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2003 ACS on STN
RN **486455-67-8** REGISTRY
CN Pentanediamide, N,N'-dibutyl-2-[(1-oxodecyl)amino]-, (2S)- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C23 H45 N3 O3
SR CA
LC STN Files: CA, CAPLUS, USPATFULL

Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

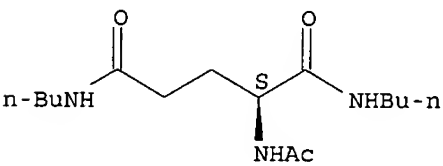
1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

=> s e7
L5 1 486455-68-9/BI

=> d

L5 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2003 ACS on STN
RN **486455-68-9** REGISTRY
CN Pentanediamide, 2-(acetylamino)-N,N'-dibutyl-, (2S)- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C15 H29 N3 O3
SR CA
LC STN Files: CA, CAPLUS, USPATFULL

Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

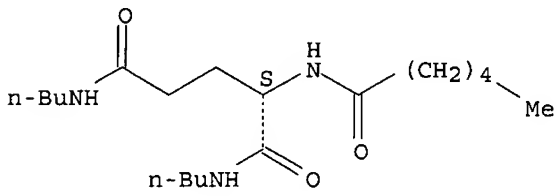
1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

=> s e8
L6 1 486455-69-0/BI

=> d

L6 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2003 ACS on STN
RN **486455-69-0** REGISTRY
CN Pentanediamide, N,N'-dibutyl-2-[(1-oxohexyl)amino]-, (2S)- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C19 H37 N3 O3
SR CA
LC STN Files: CA, CAPLUS, USPATFULL

Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

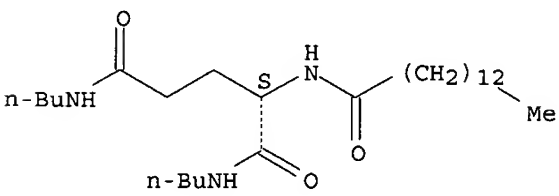
1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

=> s e9
L7 1 486455-70-3/BI

=> d

L7 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2003 ACS on STN
RN **486455-70-3** REGISTRY
CN Pentanediamide, N,N'-dibutyl-2-[(1-oxotetradecyl)amino]-, (2S)- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C27 H53 N3 O3
SR CA
LC STN Files: CA, CAPLUS, USPATFULL

Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

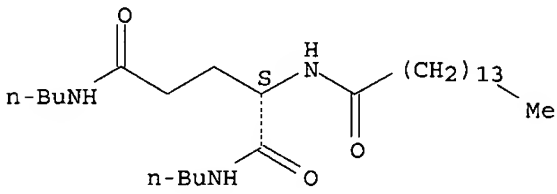
=> s e10

L8 1 486455-71-4/BI

=> d

L8 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2003 ACS on STN
RN **486455-71-4** REGISTRY
CN Pentanediamide, N,N'-dibutyl-2-[(1-oxopentadecyl)amino]-, (2S)- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C28 H55 N3 O3
SR CA
LC STN Files: CA, CAPLUS, USPATFULL

Absolute stereochemistry.

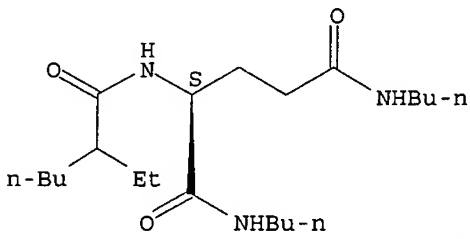


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L2 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2003 ACS on STN
RN **486455-65-6** REGISTRY
CN Pentanediamide, N,N'-dibutyl-2-[(2-ethyl-1-oxohexyl)amino]-, (2S)- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C21 H41 N3 O3
SR CA
LC STN Files: CA, CAPLUS, USPATFULL

Absolute stereochemistry.



Calculated Properties (CALC)

PROPERTY (CODE)	VALUE	CONDITION	NOTE
Bioconc. Factor (BCF)	315	pH 1	(1) ACD
Bioconc. Factor (BCF)	333	pH 4	(1) ACD
Bioconc. Factor (BCF)	333	pH 7	(1) ACD
Bioconc. Factor (BCF)	333	pH 8	(1) ACD
Bioconc. Factor (BCF)	333	pH 10	(1) ACD
Boiling Point (BP)	642.0+/-50.0 deg C	760.0 Torr	(1) ACD
Enthalpy of Vap. (HVAP)	94.76+/-3.0 kJ/mol		(1) ACD
Flash Point (FP)	190.5+/-54.5 deg C		(1) ACD
Freely Rotatable Bonds (FRB)	19		(1) ACD
H acceptors (HAC)	6		(1) ACD
H donors (HD)	3		(1) ACD
Koc (KOC)	2101	pH 1	(1) ACD
Koc (KOC)	2222	pH 4	(1) ACD
Koc (KOC)	2222	pH 7	(1) ACD
Koc (KOC)	2222	pH 8	(1) ACD
Koc (KOC)	2222	pH 10	(1) ACD
logD (LOGD)	3.60	pH 1	(1) ACD
logD (LOGD)	3.62	pH 4	(1) ACD
logD (LOGD)	3.62	pH 7	(1) ACD
logD (LOGD)	3.62	pH 8	(1) ACD
logD (LOGD)	3.62	pH 10	(1) ACD
logP (LOGP)	3.622+/-0.560		(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 1	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 4	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 7	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 8	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 10	(1) ACD
Molecular Weight (MW)	383.57		(1) ACD
Vapor Pressure (VP)	2.24E-16 Torr	25.0 deg C	(1) ACD

(1) Calculated using Advanced Chemistry Development (ACD) Software Solaris V4.76 ((C) 1994-2003 ACD)

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1

AN 138:106999 CA
TI Preparation of N-acyl-L-aspartic and -glutamic acid diamides for gel compositions and cosmetics
IN Yamamoto, Naoya; Yoshihara, Hideki
PA Ajinomoto Co., Inc., Japan
SO Fr. Demande, 23 pp.
CODEN: FRXXBL
DT Patent
LA French
IC ICM C07C225-06
ICS A61K007-027; A61K007-32
CC 34-2 (Amino Acids, Peptides, and Proteins)
Section cross-reference(s): 62
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	FR 2820739	A1	20020816	FR 2002-1751	20020213
	JP 2002316971	A2	20021031	JP 2002-31820	20020208
	US 2002159961	A1	20021031	US 2002-73226	20020213
PRAI	JP 2001-35011		20010213		

AB Title amides R3CO-L-Asp(NHR1)NHR2 and R3CO-L-Glu(NHR1)NHR2 (R1, R2 are C1-C26 hydrocarbyl and R3 is C7-C10 hydrocarbyl) were prepd. for obtaining gelling agents, gel compns., and cosmetics. Thus, N-(2-ethylhexanoyl)-L-glutamic acid dibutylamide was prepd. from sodium glutamate by acylation with 2-ethylhexanoyl chloride and amidation with dibutylamine. Synthetic dibutylamides were evaluated for gelling aptitude.
ST acyl aspartic glutamic acid diamide prepn gel compn
IT Cosmetics
(gels; prepn. of N-acyl-L-aspartic and -glutamic acid diamides for gel compns. and cosmetics)
IT 63663-21-8P 486455-65-6P 486455-66-7P 486455-67-8P 486455-68-9P 486455-69-0P 486455-70-3P 486455-71-4P
RL: COS (Cosmetic use); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of N-acyl-L-aspartic and -glutamic acid diamides for gel compns. and cosmetics)
IT 109-73-9, Butylamine, reactions 111-64-8, Octanoyl chloride 760-67-8, 2-Ethylhexanoyl chloride 16177-21-2, Sodium glutamate
RL: RCT (Reactant); RACT (Reactant or reagent)
(prepn. of N-acyl-L-aspartic and -glutamic acid diamides for gel compns. and cosmetics)

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TI Preparation of N-acyl-L-aspartic and -glutamic acid diamides for gel compositions and cosmetics
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PA Ajinomoto Co., Inc., Japan
SO Fr. Demande, 23 pp.
CODEN: FRXXBL
DT Patent
LA French
IC ICM C07C225-06
ICS A61K007-027; A61K007-32
CC 34-2 (Amino Acids, Peptides, and Proteins)
Section cross-reference(s): 62
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
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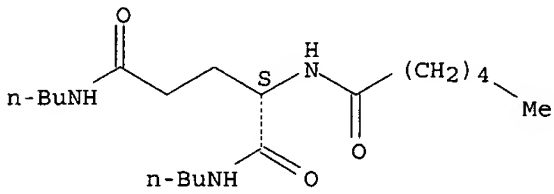
	JP 2002316971	A2	20021031	JP 2002-31820	20020208
	US 2002159961	A1	20021031	US 2002-73226	20020213
PRAI	JP 2001-35011		20010213		

AB Title amides R3CO-L-Asp(NHR1)NHR2 and R3CO-L-Glu(NHR1)NHR2 (R1, R2 are C1-C26 hydrocarbyl and R3 is C7-C10 hydrocarbyl) were prepd. for obtaining gelling agents, gel compns., and cosmetics. Thus, N-(2-ethylhexanoyl)-L-glutamic acid dibutylamide was prepd. from sodium glutamate by acylation with 2-ethylhexanoyl chloride and amidation with dibutylamine. Synthetic dibutylamides were evaluated for gelling aptitude.
ST acyl aspartic glutamic acid diamide prepn gel compn
IT Cosmetics
(gels; prepn. of N-acyl-L-aspartic and -glutamic acid diamides for gel compns. and cosmetics)
IT 63663-21-8P 486455-65-6P 486455-66-7P 486455-67-8P 486455-68-9P 486455-69-0P 486455-70-3P 486455-71-4P
RL: COS (Cosmetic use); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of N-acyl-L-aspartic and -glutamic acid diamides for gel compns. and cosmetics)
IT 109-73-9, Butylamine, reactions 111-64-8, Octanoyl chloride 760-67-8, 2-Ethylhexanoyl chloride 16177-21-2, Sodium glutamate
RL: RCT (Reactant); RACT (Reactant or reagent)
(prepn. of N-acyl-L-aspartic and -glutamic acid diamides for gel compns. and cosmetics)

L6 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2003 ACS on STN
RN **486455-69-0** REGISTRY
CN Pentanediamide, N,N'-dibutyl-2-[(1-oxohexyl)amino]-, (2S)- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C19 H37 N3 O3
SR CA
LC STN Files: CA, CAPLUS, USPATFULL

Absolute stereochemistry.



Calculated Properties (CALC)

PROPERTY (CODE)	VALUE	CONDITION	NOTE
Bioconc. Factor (BCF)	67.3	pH 1	(1) ACD
Bioconc. Factor (BCF)	71.6	pH 4	(1) ACD
Bioconc. Factor (BCF)	71.6	pH 7	(1) ACD
Bioconc. Factor (BCF)	71.6	pH 8	(1) ACD
Bioconc. Factor (BCF)	71.6	pH 10	(1) ACD
Boiling Point (BP)	632.6+/-50.0 deg C	760.0 Torr	(1) ACD
Enthalpy of Vap. (HVAP)	93.52+/-3.0 kJ/mol		(1) ACD
Flash Point (FP)	201.5+/-54.5 deg C		(1) ACD
Freely Rotatable Bonds (FRB)	18		(1) ACD
H acceptors (HAC)	6		(1) ACD
H donors (HD)	3		(1) ACD
Koc (KOC)	696	pH 1	(1) ACD
Koc (KOC)	739	pH 4	(1) ACD
Koc (KOC)	739	pH 7	(1) ACD
Koc (KOC)	739	pH 8	(1) ACD
Koc (KOC)	739	pH 10	(1) ACD
logD (LOGD)	2.72	pH 1	(1) ACD
logD (LOGD)	2.74	pH 4	(1) ACD
logD (LOGD)	2.74	pH 7	(1) ACD
logD (LOGD)	2.74	pH 8	(1) ACD
logD (LOGD)	2.74	pH 10	(1) ACD
logP (LOGP)	2.743+/-0.557		(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 1	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 4	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 7	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 8	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 10	(1) ACD
Molecular Weight (MW)	355.52		(1) ACD
Vapor Pressure (VP)	6.59E-16 Torr	25.0 deg C	(1) ACD

(1) Calculated using Advanced Chemistry Development (ACD) Software Solaris V4.76 ((C) 1994-2003 ACD)

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1

AN 138:106999 CA
TI Preparation of N-acyl-L-aspartic and -glutamic acid diamides for gel compositions and cosmetics
IN Yamamoto, Naoya; Yoshihara, Hideki
PA Ajinomoto Co., Inc., Japan
SO Fr. Demande, 23 pp.
CODEN: FRXXBL
DT Patent
LA French
IC ICM C07C225-06
ICS A61K007-027; A61K007-32
CC 34-2 (Amino Acids, Peptides, and Proteins)
Section cross-reference(s): 62
FAN.CNT 1

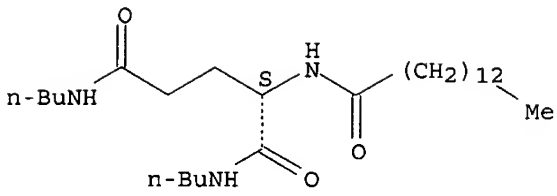
	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	FR 2820739	A1	20020816	FR 2002-1751	20020213
	JP 2002316971	A2	20021031	JP 2002-31820	20020208
	US 2002159961	A1	20021031	US 2002-73226	20020213
PRAI	JP 2001-35011		20010213		

AB Title amides R3CO-L-Asp(NHR1)NHR2 and R3CO-L-Glu(NHR1)NHR2 (R1, R2 are C1-C26 hydrocarbyl and R3 is C7-C10 hydrocarbyl) were prepd. for obtaining gelling agents, gel compns., and cosmetics. Thus, N-(2-ethylhexanoyl)-L-glutamic acid dibutylamide was prepd. from sodium glutamate by acylation with 2-ethylhexanoyl chloride and amidation with dibutylamine. Synthetic dibutylamides were evaluated for gelling aptitude.
ST acyl aspartic glutamic acid diamide prepn gel compn
IT Cosmetics
(gels; prepn. of N-acyl-L-aspartic and -glutamic acid diamides for gel compns. and cosmetics)
IT 63663-21-8P 486455-65-6P 486455-66-7P 486455-67-8P 486455-68-9P 486455-69-0P 486455-70-3P 486455-71-4P
RL: COS (Cosmetic use); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of N-acyl-L-aspartic and -glutamic acid diamides for gel compns. and cosmetics)
IT 109-73-9, Butylamine, reactions 111-64-8, Octanoyl chloride 760-67-8, 2-Ethylhexanoyl chloride 16177-21-2, Sodium glutamate
RL: RCT (Reactant); RACT (Reactant or reagent)
(prepn. of N-acyl-L-aspartic and -glutamic acid diamides for gel compns. and cosmetics)

=> d l7 all

L7 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2003 ACS on STN
RN **486455-70-3** REGISTRY
CN Pentanediamide, N,N'-dibutyl-2-[(1-oxotetradecyl)amino]-, (2S)- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C27 H53 N3 O3
SR CA
LC STN Files: CA, CAPLUS, USPATFULL

Absolute stereochemistry.



Calculated Properties (CALC)

PROPERTY (CODE)	VALUE	CONDITION	NOTE
Bioconc. Factor (BCF)	114638	pH 1	(1) ACD
Bioconc. Factor (BCF)	121519	pH 4	(1) ACD
Bioconc. Factor (BCF)	121527	pH 7	(1) ACD
Bioconc. Factor (BCF)	121527	pH 8	(1) ACD
Bioconc. Factor (BCF)	121524	pH 10	(1) ACD
Boiling Point (BP)	694.9+/-50.0 deg C	760.0 Torr	(1) ACD
Enthalpy of Vap. (HVAP)	101.78+/-3.0 kJ/mol		(1) ACD
Flash Point (FP)	167.8+/-54.5 deg C		(1) ACD
Freely Rotatable Bonds (FRB)	26		(1) ACD
H acceptors (HAC)	6		(1) ACD
H donors (HD)	3		(1) ACD
Koc (KOC)	143076	pH 1	(1) ACD
Koc (KOC)	151664	pH 4	(1) ACD
Koc (KOC)	151673	pH 7	(1) ACD
Koc (KOC)	151673	pH 8	(1) ACD
Koc (KOC)	151670	pH 10	(1) ACD
logD (LOGD)	6.97	pH 1	(1) ACD
logD (LOGD)	6.99	pH 4	(1) ACD
logD (LOGD)	6.99	pH 7	(1) ACD
logD (LOGD)	6.99	pH 8	(1) ACD
logD (LOGD)	6.99	pH 10	(1) ACD
logP (LOGP)	6.994+/-0.557		(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 1	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 4	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 7	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 8	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 10	(1) ACD
Molecular Weight (MW)	467.73		(1) ACD
Vapor Pressure (VP)	3.70E-19 Torr	25.0 deg C	(1) ACD

(1) Calculated using Advanced Chemistry Development (ACD) Software Solaris V4.76 ((C) 1994-2003 ACD)

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1

AN 138:106999 CA
TI Preparation of N-acyl-L-aspartic and -glutamic acid diamides for gel compositions and cosmetics
IN Yamamoto, Naoya; Yoshihara, Hideki
PA Ajinomoto Co., Inc., Japan
SO Fr. Demande, 23 pp.
CODEN: FRXXBL
DT Patent
LA French

IC ICM C07C225-06
ICS A61K007-027; A61K007-32
CC 34-2 (Amino Acids, Peptides, and Proteins)
Section cross-reference(s): 62
FAN.CNT 1

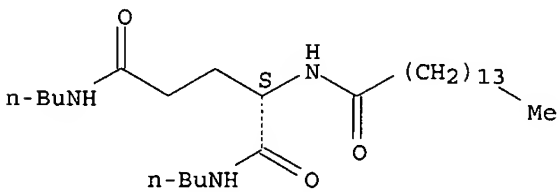
	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	FR 2820739	A1	20020816	FR 2002-1751	20020213
	JP 2002316971	A2	20021031	JP 2002-31820	20020208
	US 2002159961	A1	20021031	US 2002-73226	20020213
PRAI	JP 2001-35011		20010213		

AB Title amides R3CO-L-Asp(NHR1)NHR2 and R3CO-L-Glu(NHR1)NHR2 (R1, R2 are C1-C26 hydrocarbyl and R3 is C7-C10 hydrocarbyl) were prepd. for obtaining gelling agents, gel compns., and cosmetics. Thus, N-(2-ethylhexanoyl)-L-glutamic acid dibutylamide was prepd. from sodium glutamate by acylation with 2-ethylhexanoyl chloride and amidation with dibutylamine. Synthetic dibutylamides were evaluated for gelling aptitude.
ST acyl aspartic glutamic acid diamide prepn gel compn
IT Cosmetics
(gels; prepn. of N-acyl-L-aspartic and -glutamic acid diamides for gel compns. and cosmetics)
IT 63663-21-8P 486455-65-6P 486455-66-7P 486455-67-8P 486455-68-9P 486455-69-0P 486455-70-3P 486455-71-4P
RL: COS (Cosmetic use); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of N-acyl-L-aspartic and -glutamic acid diamides for gel compns. and cosmetics)
IT 109-73-9, Butylamine, reactions 111-64-8, Octanoyl chloride 760-67-8, 2-Ethylhexanoyl chloride 16177-21-2, Sodium glutamate
RL: RCT (Reactant); RACT (Reactant or reagent)
(prepn. of N-acyl-L-aspartic and -glutamic acid diamides for gel compns. and cosmetics)

=> d l8 all

L8 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2003 ACS on STN
RN **486455-71-4** REGISTRY
CN Pentanediamide, N,N'-dibutyl-2-[(1-oxopentadecyl)amino]-, (2S)- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C28 H55 N3 O3
SR CA
LC STN Files: CA, CAPLUS, USPATFULL

Absolute stereochemistry.



Calculated Properties (CALC)

PROPERTY (CODE)	VALUE	CONDITION	NOTE

Bioconc. Factor (BCF)	290459	pH 1	(1) ACD
Bioconc. Factor (BCF)	307892	pH 4	(1) ACD
Bioconc. Factor (BCF)	307911	pH 7	(1) ACD
Bioconc. Factor (BCF)	307911	pH 8	(1) ACD
Bioconc. Factor (BCF)	307904	pH 10	(1) ACD
Boiling Point (BP)	703.1+/-55.0 deg C	760.0 Torr	(1) ACD
Enthalpy of Vap. (HVAP)	102.90+/-3.0 kJ/mol		(1) ACD
Flash Point (FP)	163.7+/-57.0 deg C		(1) ACD
Freely Rotatable Bonds (FRB)	27		(1) ACD
H acceptors (HAC)	6		(1) ACD
H donors (HD)	3		(1) ACD
Koc (KOC)	278336	pH 1	(1) ACD
Koc (KOC)	295043	pH 4	(1) ACD
Koc (KOC)	295060	pH 7	(1) ACD
Koc (KOC)	295060	pH 8	(1) ACD
Koc (KOC)	295054	pH 10	(1) ACD
logD (LOGD)	7.50	pH 1	(1) ACD
logD (LOGD)	7.52	pH 4	(1) ACD
logD (LOGD)	7.52	pH 7	(1) ACD
logD (LOGD)	7.52	pH 8	(1) ACD
logD (LOGD)	7.52	pH 10	(1) ACD
logP (LOGP)	7.526+/-0.557		(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 1	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 4	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 7	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 8	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 10	(1) ACD
Molecular Weight (MW)	481.75		(1) ACD
Vapor Pressure (VP)	1.28E-19 Torr	25.0 deg C	(1) ACD

(1) Calculated using Advanced Chemistry Development (ACD) Software Solaris V4.76 ((C) 1994-2003 ACD)

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1

AN 138:106999 CA
TI Preparation of N-acyl-L-aspartic and -glutamic acid diamides for gel compositions and cosmetics
IN Yamamoto, Naoya; Yoshihara, Hideki
PA Ajinomoto Co., Inc., Japan
SO Fr. Demande, 23 pp.
CODEN: FRXXBL
DT Patent
LA French
IC ICM C07C225-06
ICS A61K007-027; A61K007-32
CC 34-2 (Amino Acids, Peptides, and Proteins)
Section cross-reference(s): 62
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	FR 2820739	A1	20020816	FR 2002-1751	20020213
	JP 2002316971	A2	20021031	JP 2002-31820	20020208
	US 2002159961	A1	20021031	US 2002-73226	20020213

PRAI JP 2001-35011 20010213

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